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Theory of electrostatic probe microscopy: a simple perturbative approach

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Abstract. A theoretical approach to electrostatic scanning probe microscopy is presented. We show that a simple perturbation formula, originally derived in the context of scattering theory of electromagnetic waves, can be used to obtain the capacitance and the electrostatic force between a metallic tip and an inhomogeneous dielectric sample. For inhomogeneous thin dielectric films, the scanning probe signal is shown to be proportional to the convolution between an effective surface profile and a response function of the microscope. This provides a rigorous framework to address the resolution issue and the inverse problem.

Introduction

Since the development of Scanning Tunneling Microscopy and Atomic Force Microscopy in the early eighties various techniques of Scanning Probe Microscopy (SPM) have been proposed [1], based on different local interactions between a sharp tip and the sample under study. The long range nature of electrostatic interactions makes them specially suitable to perform noncontact SPM imaging of both conducting and insulating materials. By applying a voltage between a force microscope tip and a sample, electrostatic force microscopy (EFM) has been used to study capacitance , surface potential , charge or dopant distribution, topography and dielectric properties of metallic and insulating surfaces . . . [2].

As in other SPM techniques, the interpretation of the EFM images is not always evident. Since EFM is a nonlocal technique due to the long range nature of the electrostatic interaction, the detailed shape and dimensions of the tip must then be taken into account for a precise calculation of both force and capacitance [3]. Most of the theoretical work on EFM has been focused on a better understanding of tip shape effects on the electric field, force and capacitance [4, 5]. Although the influence of the tip shape is now more or less well understood for flat and homogeneous samples, there is no simple way to directly relate the electrostatic image with the dielectric and topographic properties of the sample. In this work, we propose a theoretical approach to electrostatic probe microscopy that represents a first step to fill this gap [2]. In analogy with previous theoretical work on scanning near-field optical microscopy (SNOM) [6], we will show that the EFM image is related to both the topography and dielectric inhomogeneities of the sample through a response function which describes all the instrument properties. In the important case of imaging of thin dielectric films deposited on metallic substrates, we show that the force (or capacitance)

signal closely follows an *equivalent surface profile*. This equivalent surface profile connects the film topography with the dielectric inhomogeneities, providing a simple physical picture of the contrast mechanism in EFM.

1. Perturbative approach

We consider a three-dimensional sample with both topographic and dielectric constant inhomogeneities (see Fig. 1). This sample is a finite layer of profile $Z(x, y) = Z(\mathbf{r}_{||})$ and dielectric constant $\epsilon(\mathbf{r})$ on top of a reference sample. For simplicity, we will take a semiinfinite homogeneous ($z > 0$) substrate of dielectric constant ϵ_s as the reference sample. Our approach would equally apply to any reference sample surface with known dielectric response, however.

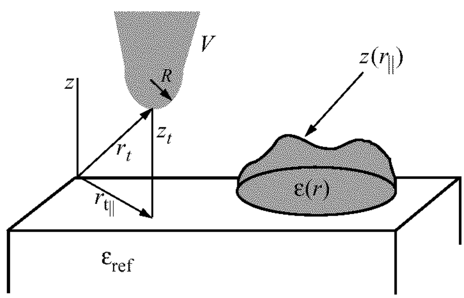

Fig. 1. Schematic configuration of an EFM.

Under a constant tip-sample bias V, the electrostatic energy of the reference system (i.e. in the homogeneous case), is given by:

$$U_0 = \frac{1}{2} \int \epsilon_0 \mathbf{E_0}^2 d^3\mathbf{r} = \frac{1}{2} C_0 V^2 \tag{1}$$

where $\mathbf{E_0}$ is the electric field and C_0 is the capacitance. The electrostatic force (normal to the sample surface) F_{0z} can be written as the energy gradient:

$$F_{0z} = -\frac{\partial}{\partial z} U_0 = -\frac{1}{2} V^2 \frac{\partial}{\partial z} C_0 \tag{2}$$

The presence of surface or volume inhomogeneities induces a change in the electrostatic energy (with respect to the reference sample),

$$\Delta U = -\frac{1}{2} \int_{\mathcal{V}} \mathbf{P} \cdot \mathbf{E_0} d^3\mathbf{r} \tag{3}$$

where $\mathbf{E_0}$ is the reference field and $\mathbf{P} = \epsilon_0(\epsilon(\mathbf{r}) - 1)\mathbf{E}$, being $\mathbf{E}$ the total field. In practice, computing the electrostatic energy (i.e. the force or/and the capacitance) from Eq. 3 requires the knowledge of the total selfconsistent field in the gap region. These are solutions of a difficult Laplace problem in an open geometry, which can only be solved numerically. In order to handle this problem we will make use of a simple perturbative approach which was shown to be useful in scattering from rough surfaces [7].

Following a simple Born-like approach one could replace the total field $\mathbf{E}$ in Eq. 3 by the nonperturbed field $\mathbf{E_0}$. However, this simple approach is known to give wrong results

in scattering from rough surfaces [7] One way to improve this approximation is to take into account the discontinuity of the normal component of the field at the boundaries [7]

$$\Delta U = -\frac{1}{2}\epsilon_0 \int_{\mathcal{V}_0} (\epsilon(\mathbf{r}) - 1) \left[\frac{E_{0z}^2}{\epsilon(\mathbf{r})} + \mathbf{E}_{0||}^2 \right] d^3\mathbf{r}. \tag{4}$$

The force signal (or the capacitance) is directly obtained from ΔU through $\Delta F = \partial \Delta U / \partial z_t$ (or $\Delta C = V^2 \Delta U / 2$). Although, in general, it is only a perturbative result, it is worth noticing that this equation gives the exact result for a parallel plate capacitor.

2. Equivalent surface profile

In order to get a deeper understanding on the nature of the image contrast, let us consider a common experimental situation in which a dielectric soft sample is on a substrate with metallic character (i.e. $\epsilon_s \to \infty$). In this case, the electric field parallel to the substrate surface will be close to zero and the main contribution to the signal will come from the normal electric field. If the dielectric thickness is small compared with a typical field gradient length scale, i.e. $E_{0z}(\mathbf{r}_{t||} - \mathbf{r}_{||}, z_t - z) \approx E_{0z}(\mathbf{r}_{t||} - \mathbf{r}_{||}, z_t)$, the energy will take the simple form of

$$\Delta U \approx \frac{1}{2}\epsilon_0 \int_{S_t} \left\{ Z_{eff}(\mathbf{r}_{||}) \cdot E_{0z}^2(\mathbf{r}_{t||} - \mathbf{r}_{||}, z_t) \right\} d^2\mathbf{r}_{||}, \tag{5}$$

where

$$Z_{eff}(\mathbf{r}_{||}) \equiv \int_0^{Z(\mathbf{r}_{||})} \frac{\epsilon(\mathbf{r}) - 1}{\epsilon(\mathbf{r})} dz \tag{6}$$

is an *equivalent surface profile* connecting the dielectric constant variation and the topography of the sample. The signal $\Delta F = \partial \Delta U / \partial z_t$ (or $\Delta C = V^2 \Delta U / 2$) will then be a simple two-dimensional convolution between the equivalent surface profile Z_{eff} and the *response function of the microscope* $\mathcal{F}(\mathbf{r}_{||}) = \partial |E_{0z}(\mathbf{r}_{||}, z_t)|^2 / \partial z_t$. Notice that the actual image would give information about Z_{eff}. For a homogeneous sample, Z_{eff} is directly proportional to the true topographic profile, while for a flat surface it reflects an average of the dielectric constant along the normal to the surface.

3. Summary

In summary, we have presented a formalism for electrostatic force microscopy based on a modified first order perturbation theory. We have checked and illustrated our theory with exact numerical results for a model system. Our model describes how the topographic and dielectric constant variations of the sample influences the observed image in EFM. This is a very important point in EFM, were the purely dielectric properties of the sample are of great interest. In analogy with SNOM imaging, we have introduced the concept of equivalent surface profile as the physical measured quantity in force microscopy. We believe that the results in this Letter should find broad applications in the analysis of electrostatic imaging with scanning probe methods.

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